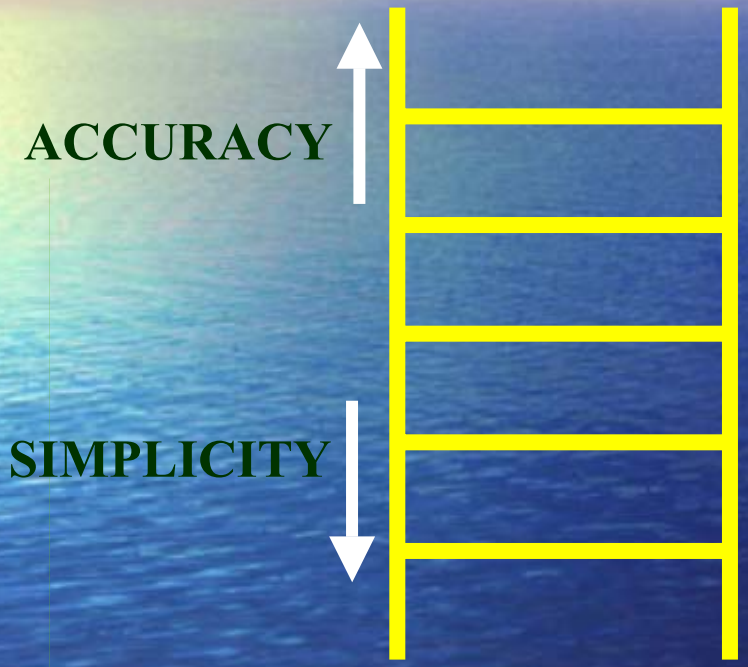
Completion of the third rung of the density functional ladder for many-electron systems



META-GENERALIZED GRADIENT APPROXIM.

GENERALIZED GRADIENT APPROXIMATION

LOCAL SPIN DENSITY APPROXIMATION

John P. Perdew, Physics, Tulane University, New Orleans

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Density functional theory permits the computer simulation of the structure of matter, including large molecules. The first three rungs of a ladder of density functional approximations have been constructed from universal exact constraints.

The third rung achieves uniform high accuracy for atoms, molecules, solids, and surfaces.

J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, Physical Review Letters 91, 146401 (2003)